REVIEWS

Journal of Semiconductors
(2021) 42, 031701
doi: 10.1088/1674-4926/42/3/031701

Low dimensional materials for photovoltaic application

Rokas Kondrotas[1, 2, ‡], Chao Chen[1, ‡], XinXing Liu[1], Bo Yang[1], and Jiang Tang[1, †]

[1]Sargent Joint Research Center, Wuhan National Laboratory for Optoelectronics and School of Optical and Electronic Information, Huazhong University of Science and Technology, Wuhan 430074, China

[2]Center for Physical Sciences and Technology, Sauletekio 3, Vilnius 10257, Lithuania

Abstract: Currently photovoltaic (PV) market is dominated by silicon based solar cells, but technology diversification is essential to promote competition which is the driving force for the technology growth. Historically, the choice of PV materials has been limited to the three-dimensional (3D) compounds with a high crystal symmetry and direct band gap. However, to meet strict demands raised for sustainable PV application, material space has been expanded beyond 3D compounds. In this perspective we discuss the potential of low dimensional materials (2D, 1D) for application in PV. We present unique features of low dimensional materials in context of their suitability in solar cells. Namely, band gap, absorption, carrier dynamics, mobility, defects, surface states and growth kinetics are discussed and compared to 3D counterparts providing a comprehensive view of prospects of low dimensional materials. Structural dimensionality leads to a highly anisotropic carrier transport, complex defect chemistry and peculiar growth dynamics. By providing fundamental insights of these challenges we aim to deepen the understanding of low dimensional materials and expand the scope of their application. In the end, we discuss the current research status and development trend of solar cell devices made of low-dimensional materials.

Key words: low dimensional materials; photovoltaic; absorption; defect; anisotropy

Citation: R Kondrotas, C Chen, X X Liu, B Yang, and J Tang, Low dimensional materials for photovoltaic application[J]. *J. Semicond.*, 2021, 42(3), 031701. http://doi.org/10.1088/1674-4926/42/3/031701

Supporting Information

1. The absorption of quasi-indirect gap materials

The absorption coefficient of the classic direct (α_{dir}) and indirect band materials (α_{ind}) can be written as:

$$\begin{aligned} \alpha_{dir} &= A_1(h\upsilon - E_{g,dir})^{1/2}, \\ \alpha_{ind} &= A_2(h\upsilon - E_{g,ind})^2. \end{aligned} \quad (S1)$$

But when we consider both direct and indirect absorption in semiconductor, the effective absorption coefficient can be written as a piecewise function:

$$\alpha_{eff} = \begin{cases} A_1(h\upsilon - E_{g,dir})^{1/2} + A_2(h\upsilon - E_{g,ind})^2, & h\upsilon > E_{g,dir}, \\ A_2(h\upsilon - E_{g,ind})^2, & E_{g,ind} \le h\upsilon \le E_{g,dir}, \\ 0, & h\upsilon < E_{g,ind}, \end{cases} \quad (S2)$$

where A_1 and A_2 are constant, $E_{g,ind}$ and $E_{g,dir}$ are the indirect and direct bandgaps. When the AM 1.5G spectrum pass through a semiconductor film with thickness of d, the absorbed photon number is given by:

$$N_{abs} = \int_{E_{g,ind}}^{+\infty} [1 - \exp(-\alpha_{eff} d)]\, \Phi_{sun} dE, \quad (S3)$$

where N_{abs} is the number of absorbed photons, Φ_{sun} is the photon density spectrum of AM 1.5G spectrum, and d is the thickness of film.

In addition, the number of photons, absorbed by the semiconductor in principle, can be written as:

$$N_{all} = \int_{E_{g,ind}}^{+\infty} \Phi_{sun} dE, \quad (S4)$$

Taking Φ_{sun}, A_1, A_2, $E_{g,ind}$, $d = 2\ \mu m$ and ΔE (defined as $E_{g,dir} - E_{g,ind}$) into the above integral equation, we can obtain the N_{abs} and N_{all}. Obviously, N_{abs}/N_{all} is a function of $E_{g,ind}$ and ΔE.

2. The ratio of N_{ind} to N_{total}

Firstly, we rely on the two assumptions: i) The electron effective mass (m_e*) of ICBM (indirect conduction band minimum) is the same as that of DCBM (direct conduction band maximum); ii) The energy dispersion relations at ICBM and DCBM meet parabola approximation.

The density of states is given by:

$$\begin{cases} g_{ind}(E) = A(E - E_{ICBM})^{1/2}, \\ g_{dir}(E) = A(E - E_{DCBM})^{1/2}, \end{cases} \quad (S5)$$

where A is a constant related to effective mass ($A = \frac{V}{2\pi^2}\frac{(2m_e^*)^{3/2}}{\hbar^3}$). The electron distribution is described by Fermi-Dirac distribution as:

$$f(E) = \frac{1}{1 + \exp\left(\frac{E - E_{ICBM}}{kT}\right)}, \quad (S6)$$

Thus the electron number on ICBM is:

$$N_{ind} = \int_{E_{ICBM}}^{+\infty} g_{ind}(E) f(E) dE. \quad (S7)$$

Take Eqs. (S5) and (S6) into Eq. (S7)

Rokas Kondrotas and Chao Chen contributed equally.

Correspondence to: J Tang, J Tang, jtang@mail.hust.edu.cn

Received 4 AUGUST 2020; Revised 27 SEPTEMBER 2020.

©2021 Chinese Institute of Electronics

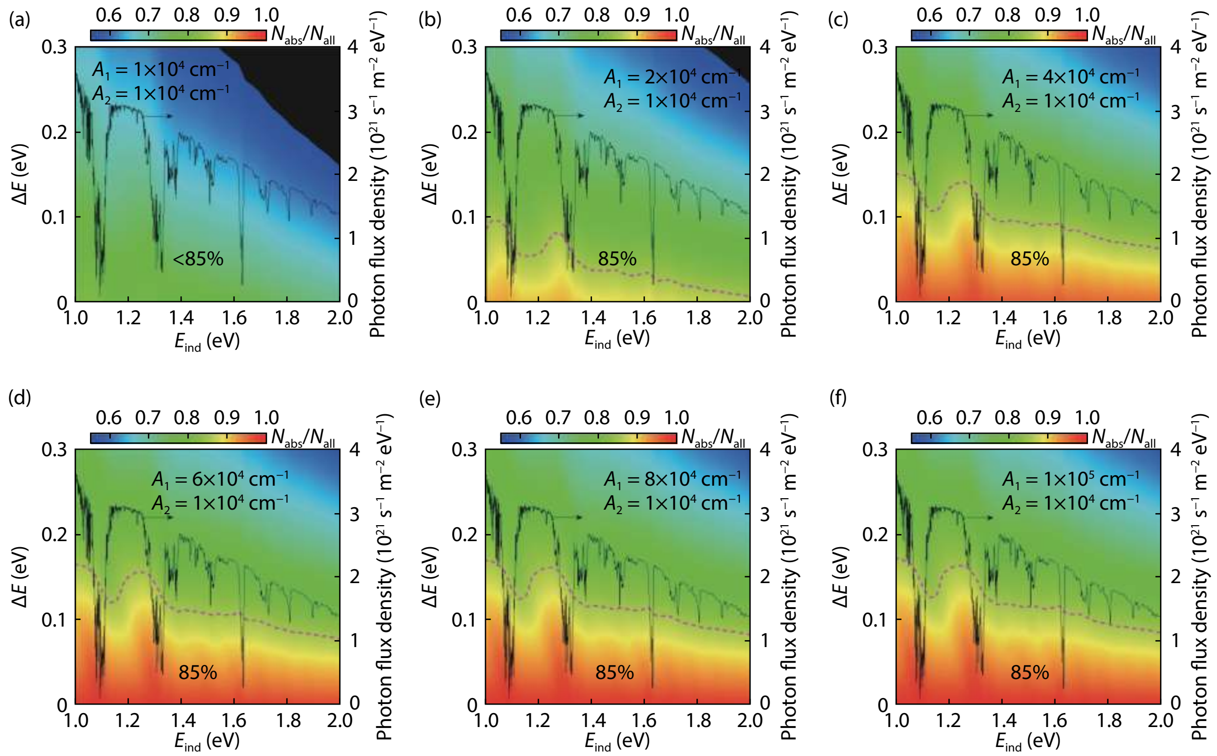

Fig. S1. (Color online) Fix A_2 as 10^4 cm^{-1} and scan A_1 from 10^4–10^5 cm^{-1}

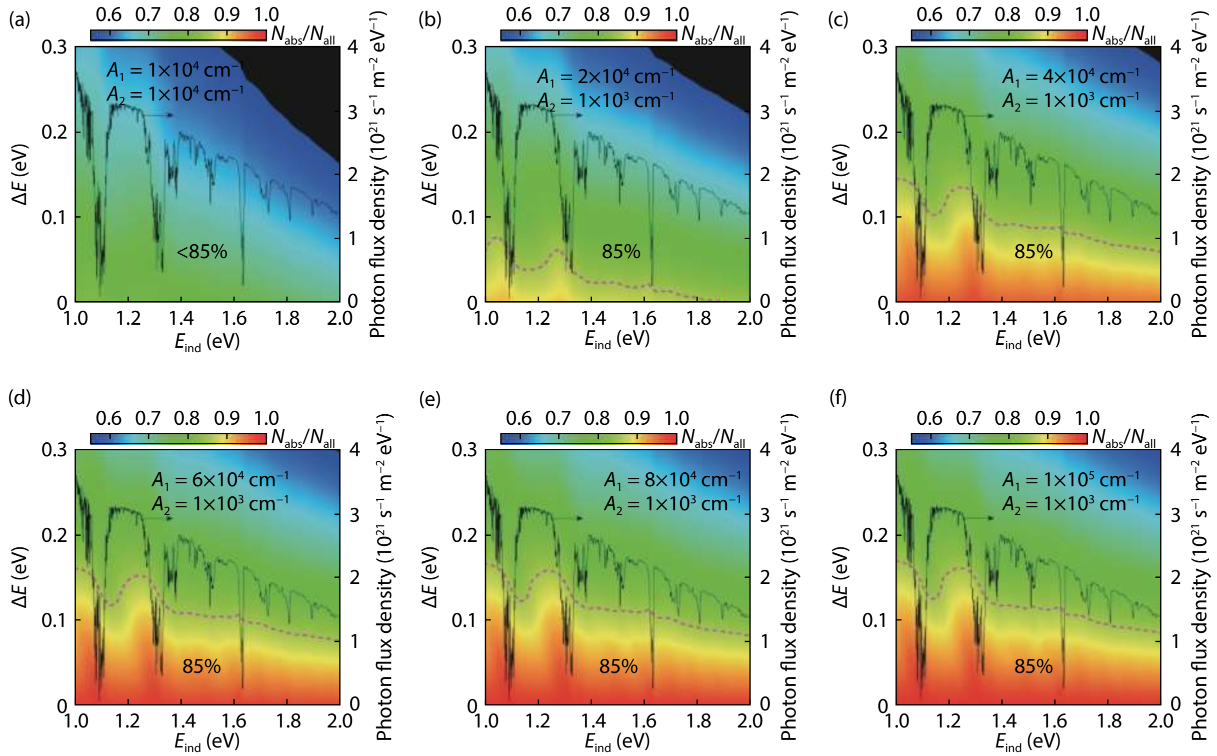

Fig. S2. (Color online) Fix A_2 as 10^3 cm^{-1} and scan A_1 from 10^4–10^5 cm^{-1}

$$\begin{cases} N_{\rm ind} = \displaystyle\int_{E_{\rm ICBM}}^{+\infty} \frac{A(E-E_{\rm ICBM})^{1/2}}{1+\exp\left(\dfrac{E-E_{\rm ICBM}}{kT}\right)}{\rm d}E, \\ N_{\rm dir} = \displaystyle\int_{E_{\rm DCBM}}^{+\infty} \frac{A(E-E_{\rm DCBM})^{1/2}}{1+\exp\left(\dfrac{E-E_{\rm ICBM}}{kT}\right)}{\rm d}E. \end{cases} \tag{S8}$$

Here we consider the intrinsic semiconductor, indicating $E - E_{\rm ICBM} >> kT$.

$$\begin{cases} N_{\rm ind} = \displaystyle\int_{E_{\rm ICBM}}^{+\infty} A(E-E_{\rm ICBM})^{1/2}\exp\left(-\frac{E-E_{\rm ICBM}}{kT}\right){\rm d}E, \\ N_{\rm dir} = \displaystyle\int_{E_{\rm DCBM}}^{+\infty} A(E-E_{\rm DCBM})^{1/2}\exp\left(-\frac{E-E_{\rm ICBM}}{kT}\right){\rm d}E. \end{cases} \tag{S9}$$

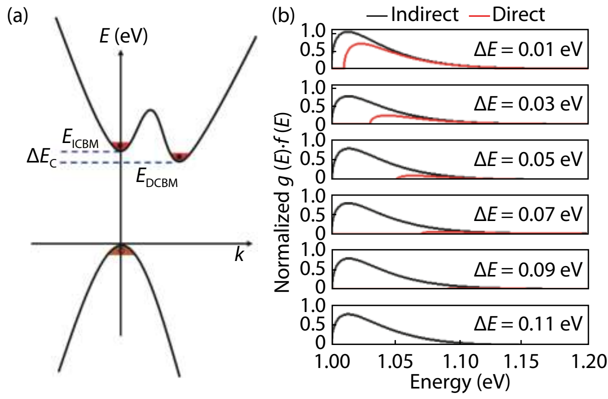

Fig. S3. The ratio of N_{ind} to N_{total} carrier dynamics. (a) The schematic diagram of energy dispersion relations at ICBM and DCBM. (b) The $g(E)\cdot f(E)$ of indirect and direct conduction bands as a function of energy. The area of curves with x-axis is proportional to the electron number. As the ΔE increase from 0.01 to 0.11 eV, the electron number at DCBM reduce exponentially

Set $x = (E - E_{ICBM})/kT$. Using $E_{DCBM} - E_{ICBM} = \Delta E$, Eq. (S9) can be written as:

$$\begin{cases} N_{ind} = A(kT)^{1/2}\int_0^{+\infty} x^{1/2}\exp(-x)\mathrm{d}E, \\ N_{dir} = A(kT)^{1/2}\exp(-\Delta E/kT)\int_0^{+\infty} x^{1/2}\exp(-x)\mathrm{d}E. \end{cases} \tag{S10}$$

Using the integration formula of $\int_0^{+\infty} x^{1/2}\exp(-x)dx = \sqrt{\pi}/2$, we can get:

$$\begin{cases} N_{ind} = \dfrac{A(\pi kT)^{1/2}}{2}, \\ N_{dir} = \dfrac{A(\pi kT)^{1/2}}{2}\exp(-\Delta E/kT). \end{cases} \tag{S11}$$

So the ratio of N_{ind} to N_{total} ($N_{ind} + N_{dir}$) is:

$$\frac{N_{ind}}{N_{total}} = \frac{1}{1+\exp(-\Delta E/kT)} \tag{S12}$$

Fig. 2(c) is the plot of N_{ind}/N_{total} as function of ΔE and temperature.

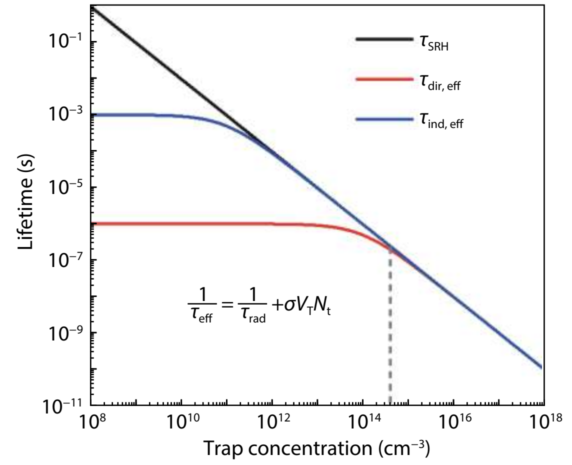

Fig. S4. (Color online) The effective carrier lifetime. When the trap density is < 3×10^{14} cm^{-3}, the indirect bandgap materials can still maintain longer effective lifetime than direct bandgap materials

3. The effective carrier lifetime

Considering the effect of defect-assistant (Shockley-Read-Hall) recombination, the effective lifetime (τ_{eff}) can be calculated by:

$$\frac{1}{\tau_{eff}} = \frac{1}{\tau_{rad}} + \frac{1}{\tau_{SRH}}, \tag{S13}$$

where τ_{rad} is the radiation lifetime, τ_{SRH} is the Shockley-Read-Hall recombination lifetime. The τ_{rad} of indirect and direct bandgap materials are usually ~ 1 and ~ 1 μs, respectively. τ_{SRH} is given by:

$$\tau_{SRH} = \frac{1}{\sigma V_T N_t}, \tag{S14}$$

where σ is the capture cross section, V_T is the thermal rate as 10^7 cm/s and N_t is the trap concentration. In high-efficient solar cells, σ is always below 10^{-15} cm^2. Taking these parameters into Eq. (S13), the τ_{eff} as a function of trap concentration is shown in Fig. S4. When the trap density is < 3×10^{14} cm^{-3}, the indirect bandgap materials can still maintain longer effective lifetime than direct bandgap materials.